Ge_n

Ge_n^+

Ge_n^+

D_0

ВФ - А.303

Drowart J. и др. 1959
J. Chem. Phys., 512
30, N1, 308

Масс-спектрометрическое изучение соединений, состоящих из эл-тов группы IV B.

1967
102

Ge_n

$n = 2, 3, 4$

Ф.о.

Goldfinger P.

La chimica e l'industria, 49, №1, 51.

Химическая и физическая устойчивость простых газообразных молекул.

Ge+ Эм. связи, стаб. гибрид

50606.430 Ph,MGU,TC	Ge$_n^-$ 7623 (Ae$^-$) (стаб. гибрид)	1975 КЧ-8980

Leleyter M., M[lle], Joyes P. Etude expé - rimentale et théorique de l'émission secondaire d'ions molécualaires. ▮ cas des éléments du groupe IV-B. "J. phys." (France), 1975, 36, № 5, 343-355 (франц., рез. англ.) 0381 пик

361 361 373 ВИНИТИ

Ge_9^{4-}

Ge_9^{2-}

1981

95: 209915h Relativistically parameterized extended-Hueckel calculations. 5. Charged polyhedral clusters of germanium, tin, lead, and bismuth atoms. Lohr, Lawrence L., Jr. (Dep. Chem., Univ. Michigan, Ann Arbor, MI 48109 USA). *Inorg. Chem.* 1981, 20(12), 4229–35 (Eng). Relativistically parameterized extended-Hueckel (REX) calcns. are reported for the homonuclear clusters Ge_9^{4-}, Ge_9^{2-}, Sn_4^{2-}, Sn_5^{2-}, Sn_9^{4-}, Pb_5^{2-}, Pb_9^{4-}, and Bi_9^{5+}, the heteronuclear clusters $PbSn_4^{2-}$, $SnGe_8^{4-}$, $GeSn_8^{4-}$, $PbSn_8^{4-}$, and $TlSn_8^{5-}$, and the exopolyhedral cluster $CH_3Pb_9^{3-}$. The reported results include binding energies per atom, rearrangement energies, and charge distributions. Significant differences are found for the heavier element clusters between the results obtained by using the relativistic parameterization and those obtained by using the nonrelativistic parameterization. Relativistic effects appear to reduce the binding energy per atom in homonuclear clusters and to alter the charge distributions in the heteronuclear clusters AB_8^{q-}. The latter effects are discussed in terms of relativistic effects on the variation of at. electronegativity with at. charge.

теорем. расчет

(+12)

C. A. 1981, 95, N24

Ge_n (кластеры)

$n=3,4,5,7,9$

1982

13 Б48. **Химические применения топологии и теории групп. 12. Кластеры постпереходных элементов, в частности, системы с девятью вершинами.** King R. Bruce. Chemical applications of topology and group theory. 12. Post-transition element clusters with particular emphasis on nine vertex systems. «Inorg. chim. acta», 1982, 57, № 1, 79—86 (англ.)

Качественные концепции двумерной и трехмерной ароматичности применены к анализу структуры и числа кластерных электронов в кластерах постпереходных элементов (Ge, Sn, Pb, Sb, Bi, Se, Te), содержащих 3, 4, 5, 7 и 9 атомов. Обсуждены условия трехмерной делокализации кластерных электронов и резонансной стабилизации трехмерных кластерных структур, связанные с понятием трехмерной ароматичности, и на основе теории графов выявлена топологич. природа правила $(2n+2)$ кластерных электронов. Рассмотрены примеры тригонально-бипирамидальных кластеров с 12 скелетны-

(+6) Sn_n .....

Ж. 1982, 19, №13.

ми электронами, к к-рым применима модель связей, локализованных вдоль ребер, 9-атомных кластеров, подчиняющихся правилу $(2n+2)$ и отклоняющихся от него и т. д. По резюме

$GeCl_2$ - 1983

O'Neill M.E., Wade K.

Polyhedron, 1983, 2,

Re; N 9, 963-966.

(cm. B_3Cl_9; III)

без

Оп. 16950

1983

классов

Pacchioni G., Plavsic D., et al.

Z=3-6

Ber. Bunsenges. phys. Chem., 1983, 87, N6, 503-512.

хим.-свеж, электрон. спектр.

Ge$_x$ 1984

Frober F.W., Schulze W.

Surface Sci., 1985, 156, N2: Small Part. and Inorg. Clusters. Proc. 3rd Int. Meet., Berlin (West), 9-13 July, 1984. Pt2, 765-769.

(См. Ge$_2$; III)

спектр,

Di, структ.

Be m.
(m=3-6)

Оп. 19027

1984

Pacchioni G., Koutecky J.;
Ber. Bunsenges. Phys.
Chem., 1984, 88, N 3,
242-245.

Электрон. структура, геометрия

бех

Ом. 23821

1985

Martin T. P., Schaber H.,

J. Chem. Phys. 1985,

83, N 2, 855–858.

Кластерн. ионн спектр-ры, спав. $x \leq 25$

Ge_{π}^{3+}

1986

Joyes P., Van de Walle J., et al.

Ultramicroscopy 1986, 20 (1-2), 65-70.

( сер. Sn_{π}^{3+}; III)

Ge_8

1986

Joyes P., Van de Walle J., et al.

ешабиевн.
структ.

Ultramicroscopy 1986, 20 (1-2), 65-70.

(см. Sn_n^{3+}; III)

Бет (от 24396) 1986

№2 Koutecky J., Fantucci P.,

Chem. Rev., 1986, 86,
N3, 539-587.

теорет.
расчет
структ.
и энергет.

бет

рт. 23761

1986

Pacchioni G., Koutecky J.,

Энергия возб. и спектр. теор. расч

J. Chem. Phys., 1986, 84, N 6, 3301–3310.

Ge_n^+ (Dm. 26198) 1986

Phillips J.C.,

J. Chem. Phys., 1986, 85, N9,

5246 - 5250.

бел

Оп. 23699

1986

п≤7

Reents W.D., Bondybey V.E.,

Chem. Phys. Lett.,

1986, 125, №4, 324–327.

лазерн. испарен., масс-спектр.

бен (см. 27242) 1987

(n=3-7) Cheshnovsky O., Yang S.-H., et al.,

фотоэлектр-спектр Chem. Phys. Lett., 1987, 138, N2-3, 119-124.

Ge_m 1987

$m = 3 \div 7$ Pacchioni Gianfranco,
Koutecky Jaroslav.

эл. . NATO ASI Ser., Ser. B
структ. 1987, 158, 439-44.

(сер. Ст, III)

Be_n

$Be_n^{+,-}$

(ОМ-27684) 1987

Phillips J. C.

J. Chem. Phys., 1987, 87, N 3, 1712–1716.

структура, теор.-расчёт

бп

1987

109: 200470j Mass and temperature measurement in pure vapor expansion of metals and semi-metals. Pruett, J. G.; Windischmann, H.; Nicholas, M. L.; Lampard, P. S. (Standard Oil Co., Cleveland, OH 44128 USA). *NATO ASI Ser., Ser. B* 1987, 158(Phys. Chem. Small Clusters), 109–14 (Eng). Mass spectrometric measurement in combination with temp. measurement of a pure-vapor source indicate that the expanding gas is rotationally cooled to ~130 K but not substantially vibrationally cooled. The data indicate that while small clusters are present for several different materials, no large clusters were produced for a source operated under a wide variety of conditions. Large Ge and Si clusters were obsd. in a laser vaporization gas aggregation source.

лазерное испарение

(Ge) IX Si

C.A. 1988, 109, N 22.

Кластеры + бер (Оп. 27766) 1987

Schulze W., Winter B., et al.,

стабильн. Z. Chem. Phys., 1987, 87, N4, 2402-2403.

Generation of germanium clusters using the gas aggregation

technique: Stability of small charged clusters.

1987

Ge n

Srowa W. Z., Freeman R. R., et al.

обзор Science, 1987, 235, N4791, 860–865.

(см. Cn; III)

бет

1988

Ом 30180

n=2÷14

109: 80018u Ground-state and finite-temperature energetics and topologies of germanium microclusters. Antonio, Gional A.; Feuston, Bradley P.; Kalia, Rajiv K.; Vashishta, P. (Inst. Fis. Quim., Univ. Sao Paulo, 13560 Sao Carlos, Brazil). *J. Chem. Phys.* 1988, 88(12), 7671–86 (Eng). The ground-state and finite-temp. properties of Ge microclusters (N = 2 to 14) were investigated by using mol. dynamics simulation along with the method of steepest-descent quench. Results indicate that the exptl. obsd. greater stability of certain cluster sizes can be explained by the topol. and energetics of the clusters at finite temp. rather than by the binding energies of the ground-state structures.

спавинн. расчет

C. A. 1988, 109, N 10

Ge

1988

110: 199495h Many-body perturbation theory applied to small germanium clusters. Islam, M. S.; Ray, A. K. (Dep. Phys., Univ. Texas, Arlington, TX 76019 USA). *Chem. Phys. Lett.* 1988, 153(6), 496–502 (Eng). Accurate ab initio mol.-orbital calcns. are performed for small germanium clusters. Many-body perturbation theory was used to study the effects of electron correlation. Results were compared with available theor. and exptl. data.

ab initio расчет

C.A. 1989, 110, N22

Be_n
$n = 3-7$

структура, До, расчет.

Erkoc S.

1991

Z. Phys. D: At., Mol clusters 1991, <u>19</u>(1-4), 423-5.

(См. C_n $n=3-7$; <u>III</u>)

Be (кластери)

Om 36692

1992

Boča R., Hajko P., et al.,

Czechoslovak Journal of Physics, 1992, 42, N7, 685-694

Molecular orbital study of Germanium, ber manium - bal-

lium and bismarium - Arsenic
Clusters.

Ge n

n = 2 ÷ 6

1993

119: 279254e Geometries and energies of small germanium (Ge_n; n = 2–6) clusters: an ab initio molecular orbital study. Lanza, Giuseppe; Millefiori, Salvatore; Millefiori, Arcangelo; Dupuis, Michel (Dip. Sci. Chim., Univ. Catania, 95125 Catania, Italy). *J. Chem. Soc., Faraday Trans.* 1993, 89(16), 2961–7 (Eng). The mol. geometries and relative stabilities of various electronic configurations of Ge_n clusters (n = 2–6) have been investigated by means of ab initio calcns. by employing an effective core potential for core electrons and a double zeta plus polarization functions basis set for valence electrons. The calcns. have produced the following optimal configurations: Ge_2 ($D_{\infty h}$, $^3\Sigma_g^-$), Ge_3 (equilateral triangle, D_{3h} $^3A'_2$), Ge_4 (planar rhombus D_{2h} ^1A_g), Ge_5 (oblate distorted trigonal bipyramid, D_{3h} $^1A'_1$), Ge_6 (edge-capped trigonal bipyramid, C_{2v} $^1A_1$). Binding energies have been evaluated by single-point (CISD(Q) calcns. at the SCF optimal ground-state geometry of the clusters. The results are in qual. agreement with exptl. data. The comparison of Ge_n and Si_n properties shows close similarity between Ge and Si.

структура, свойства, теор. расчет

С. А. 1993, 119, N26.

Ge 60

1994

Slanina Z.,
Lee Shyi-Long.
Fullerene Sci. Technol. 1994, 2 (4), 453-69.
(Данные.)

(сеч. C_{60} ; III)

Ge5 Дай Д. 1996

125: 257579m **Geometries and energy separations of 28 electronic states of Ge_5.** Dai, Dingguo; Balasubramanian, K. (Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287–1604 USA). *J. Chem. Phys.* **1996**, 105(14), 5901–5906 (Eng). Geometries and energy sepns. of 28 low–lying electronic states of Ge_5 with different structures (trigonal bipyramid, D_{3h}; edge–capped tetrahedron, C_{2v}; tetragonal pyramid, C_{4v}; planar square, D_{4h}; planar pentagon, D_{5h}' linear, $D_{\infty h}$; and tetrahedron, T_d) are investigated in this study. We employ the complete active space multiconfiguration self–consistent–field method (CAS–SCF) followed by large scale multireference singles + doubles CI (MRSD–CI) computations that included up to 3.86 million configurations. Atomization and dissocn. energies of Ge_5 are computed and compared with smaller clusters.

структура и энергии низших эл. состоян., теор. расчет

Е. А. 1996, 125, N 20

бер

1997

n = 2-5

127: 100077q **Binding energies of germanium clusters, Ge_n (n = 2–5).** Deutsch, P. W.; Curtiss, L. A.; Blaudeau, J. P. (Department of Physics, Pennsylvania State University, Monaca, PA 15061 USA). *Chem. Phys. Lett.* **1997**, 270(5,6), 413–418 (Eng), Elsevier. Gaussian–2 (G2) theory for third–row non–transition elements is used to calc. energies of germanium clusters, Ge_n (n = 2–5). The G2 energies are used to derive accurate binding energies for the clusters. The results for Ge_2 and Ge_3 are in agreement with expt. while there is some disagreement for Ge_4 and Ge_5. The binding energies are also calcd. using the B3LYP d.–functional method with the 6–311+G(3df,2p) basis set and compared with the G2 results and expt.

(энергия связи, теор. расч.)

C. A. 1997, 127, N 7

Ge_n^-
Ge_n
$n = 2 \div 6$

1998

129: 166429d **A study of Ge_n^- and Ge_n (n = 2–6) using B3LYP–DFT and CCSD(T) methods: the structures and electron affinities of small germanium clusters.** Archibong, Edet F.; St–Amant, Alain (Department of Chemistry, University of Ottawa, 10 Marie Curie Street, Ottawa, ON Can. K1N 6N5). *J. Chem. Phys.* 1998, 109(3), 962–972 (Eng), American Institute of Physics. The structures of the anionic germanium Ge_n^- clusters and the corresponding neutral Ge_n clusters (n = 2–6) have been investigated using B3LYP–DFT and CCSD(T) methods. The 6–311+G(3df) basis set is employed for the dimers and trimers, while the smaller 6–311+G(d) basis set is used for clusters with n > 3. The most stable structures for the germanium cluster anions Ge_3^-, Ge_4^-, Ge_5^-, and Ge_6^- are found to be $C_{2v}(^2A_1)$, $D_{2h}(^2B_{2g})$, $D_{3h}(^2A_2")$, and $D_{4h}(^2A_{2u})$, resp. In the case of Ge_2^-, our calcns. show that the low lying $^2\Pi_u$ and $^2\Sigma_g^+$ states are within 1 kcal/mol of each other and both states are candidates for the ground state of the anion. The adiabatic electron affinities calcd. for the Ge_n clusters with n = 2, 3, 4, 6 are within 0.1 eV of the corresponding exptl. values. Furthermore, the adiabatic excitation energies computed at the CCSD(T) level for the low lying states of Ge_3 and Ge_4 compare quite well with the assignments of the bands obsd. in the photoelectron spectra of Ge_3^- and Ge_4^- by Burton, Xu, Arnold, and Neumark [J. Chem. Phys. 104, 2757 (1996)].

структура, Ае, теор. расчет

CA1998, 129, W13

Ge_5^+

1998

128: 286597h **Geometries and energy separations of the electronic states of Ge_5^+ and Sn_5^+.** Dai, Dingguo; Balasubramanian, K. (Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287–1604 USA). *J. Chem. Phys.* 1998, 108(11), 4379–4385 (Eng), American Institute of Physics. We compute the geometries and energy sepns. of 13 low–lying electronic states of Ge_5^+ and Sn_5^+ with five different structures (edge–capped tetrahedron, C_{2v}; trigonal bipyramid, D_{3h}; tetragonal pyramid, C_{4v}; planar square, D_{4h}; and planar pentagon, D_{5h}). The complete active space multiconfiguration self–consistent–field method (CAS–SCF) followed by large scale multireference singles + doubles CI (MRSD–CI) computations that included up to 3.77 million configurations are employed. It was found that upon ionization the sym. D_{3h} trigonal bipyramidal structures of Ge_5 and Sn_5 Jahn–Teller distort into nearly degenerate $^2B_2$ and $^2A_1$ electronic states with edge–capped tetrahedral (C_{2v}) geometry. Atomization and dissocn. energies of Ge_5^+ and Sn_5^+ as well as adiabatic ionization energies of Ge_5 and Sn_5 are computed.

стр-ра и стабильн., энер. расчёт

(+) Sn_5^+ □

C.A. 1998, 128, N23

Clx

On. 40021

1999

Vicki D Morarec et al.,

Ae J. Chem. Phys. 1999,

110, N11, 5079

Фуллерен
C60

1999

Leszczynski, Jerzy; et al.,

потенц. ионизац. теорет. расчет

J. Phys. Chem. A 1999, 103 (3), 396-401

(см. C60; фуллерен III)

бет

n=2-13

(Ом. 40458)

2000

Chulsu Jo and Keejung Lee,

J. Chem. Phys., 2000,

113, N17, 7268-7272

Semiempirical tight binding

method study of
small be and in clusters

1999

F: Gen
P: 3
131:314355 Structures of Germanium Clusters: Where the Growth Patterns of Silicon and Germanium Clusters Diverge. Shvartsburg, Alexandre A.; Liu, B Lu, Zhong-Yi; Wang, Cai-Zhuang; Jarrold, Martin F.; Ho, Kai-Ming Departme Chemistry, Northwestern University Evanston, IL 60208, USA Phys. Rev. Let 83(11), 2167-2170 (English) 1999. We have performed a systematic ground state geometry search for Gen neutrals and cations in the

n .ltoreq. 16 size range using d. functional local d. approxn. and gradient-cor. methods. Like their silicon analogs, medium-sized Ge clusters are stacks of tricapped trigonal prism subunits. However, the structures of Gen and Sin for n = 13 and n .gtoreq. 15 diffe details. The onset of the structural divergence between the growth patte Si and Ge clusters is confirmed by the measurements of gas phase ion mobi fragmentation pathways, and dissocn. energies.

бето

2000

смад. структ. теорет. данет

133: 140552w **Stable structures for Ge_{10} cluster and comparative study with Si_{10} cluster.** Li, Bao-Xing; Cao, Pei-Lin (Department of Physics and State Key Laboratory of Silicon Material, Zhejiang University, Hangzhou, Peop. Rep. China 310027). *Phys. Status Solidi B* 2000, 219(2), 253-266 (Eng), Wiley-VCH Verlag Berlin GmbH. Full-potential linear-muffin-tin-orbital mol.-dynamics (FP-LMTO MD) calcns. have been performed to investigate the structures and energies of small cluster Ge_{10}. We get twenty three stable structures for Ge_{10}. The results suggest that only five structures are stable among the six structures proposed before, the remainder undergoes a distortion to another more stable form. Making comparison with the structures of Si_{10} cluster, we find that there are much in common between them. But their ground state structures are different.

C. A. 2000, 133, N10

2000

F: Gen
P: 3

134:317825 **Photoionization and Photodissociation studies of semiconductor clusters.** Yoshida, Shinji; Fuke, Kiyokazu. Department of Chemistry, Kobe University, Kobe, Japan. Trans. Mater. Res. Soc. Jpn. (2000), 25(4), 995-998. in English.

Photoionization thresholds for Gen ($n \leq 57$) and Snn ($n \leq 41$) were studied with detection by reflectron time-of-flight mass spectrometry. Stimulated Raman scattering lights of narrow bandwidth UV radiation were used as the ionization light source in the vacuum UV region (200-141 nm). A very similar

size dependence of ionization potentials (IPs) is found for Gen and Snn with <12 atoms. The authors also find a rapid decrease in IPs for Gen between n = 15 and 26, which is similar to that for Sin found in the authors' previous work. However, the IPs of Snn (n = 15-41), which is metallic in bulk solid at room temp., decrease slowly without a gap. The difference in the size dependence of IPs for the medium size Si Ge and Snn clusters is discussed in relation to the existence of a structural transition. The authors have also examd. the photodissocn. process of Snn+ clusters. The authors observe a trend for the evapn. of atom and/or dimer, which is usually obsd. for metal clusters, in addn. to a fission-type fragmentation as is obsd. for Sin+ and Gen+.

Ge_6, Ge_6^+, Ge_6^- | Dm. 41003 | 2271

Cunyuan Zhao et al.,

Economou, Chem. Phys., 2001,
Chem. 115, N7, 8121...
Ge-Ge

Geometries and properties and tin

spectroscopic of germanium hexamers (Ge_6,

$\delta\varepsilon^+$, $\delta\varepsilon^-$, $\mathcal{L}_{n6}$, $\mathcal{L}_{n6}^+$, или $\mathcal{L}_{n6}^-$).

Ge_n^-
$n = 2-5$

2001

(Ae, теор. расч.)

135: 377058u **Electron affinities of germanium anion clusters, Ge_n^- (n = 2–5).** Deutsch, P. W.; Curtiss, L. A.; Blaudeau, J.-P. (Department of Physics, Pennsylvania State University, Monaca, PA 15061 USA). *Chem. Phys. Lett.* **2001**, 344(1,2), 101–106 (Eng), Elsevier Science B.V. Gaussian–2 (G2) theory for third–row non–transition elements is used to calc. accurate electron affinities of germanium clusters, Ge_n (n = 2–5). The results for n = 2–4 are in agreement with expt. while there is some disagreement for Ge_5. The electron affinities are also calcd. using G2 theory modified by adding a diffuse function to the basis set for MP2 geometry optimizations and using the B3LYP d. functional method with the 6–311+G(3df,2p) basis set.

C.A. 2001, 135, N26

Ln

n = 5-10

Om. 41180

2001

Si-Dian Li et al.,

J. Chem. Phys., 2001,

115, N20, 9255-9259.

Ionization potentials, electron affinities, and vibrational

frequencies of for ($n=5-10$)
neutrals and charged ions
from density functional
theory.

Ge_6, Ge_6^+, Ge_6^- 2001

135: 335341a **Geometries and spectroscopic properties of germanium and tin hexamers (Ge_6, Ge_6^+, Ge_6^-, Sn_6, Sn_6^+, and Sn_6^-).** Zhao, Cunyuan; Balasubramanian, K. (Department of Applied Science, L−794, University of California Davis, Livermore, CA 94550 USA). *J. Chem. Phys.* 2001, 115(7), 3121−3133 (Eng), American Institute of Physics. Ground and excited electronic states of neutral, cationic and anionic germanium and tin hexamers (Ge_6 and Sn_6) are investigated. Different geometries such as tetragonal bipyramid (D_{4h},D_{2h}) and edge−capped trigonal bipyramid (C_{2v}) (ECTBP) were studied. We have employed a no. of high level electron correlation techniques such as large scale multireference singles+doubles CI (MRSDCI) computations that included up to 16 million configurations, complete active−space multiconfiguration self−consistent filed (CAS−MCSCF), and Moller−Plesset (MP2) techniques to investigate the low−lying electronic states, their geometries and energy sepns. A $^1A_{1g}$ tetragonal bipyramid structure (D_{4h} symmetry) is found as the ground state for both Ge_6 and Sn_6, in accord with

структура, м.х., теор. расчет.

(+) □

С.А. 2001, 135, N23

Sn_6, Sn_6^+, Sn_6^-

the previously suggested exptl. assignments. The excitation energies, atomization energies, ionization potentials and vertical and adiabatic electron affinities are computed and compared with the exptl. results. Our computations of the excited states of these species have facilitated assignment of the anion photodetachment spectra of the anions of these clusters and comparison with the photoionization spectra of the neutral species.